

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.62e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.76e-01

Confidence level: 3.95e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>alpha-Santonin</div> <div>Measured: 8.12e-04</div> <div>Predicted: 5.45e-04</div>	<div>Image not found</div> <div>Oxabentrinil</div> <div>Measured: 8.61e-05</div> <div>Predicted: 1.53e-03</div>	<div>Image not found</div> <div>.alpha.- [(Cyanomethoxy)imino]benzeneacetonitrile</div> <div>Measured: 5.13e-04</div> <div>Predicted: 5.60e-02</div>
<div>Image not found</div> <div>Siduron</div> <div>Measured: 7.75e-05</div> <div>Predicted: 2.20e-03</div>	<div>Image not found</div> <div>Benquinox</div> <div>Measured: 2.07e-05</div> <div>Predicted: 3.02e-02</div>	